

Optimal Control-Based Efficient Synthesis of Building Blocks of Quantum Algorithms Seen in Perspective from Network Complexity towards Time Complexity*

T. Schulte-Herbrüggen[†] and A. Spörl

*Department of Chemistry, Technical University Munich,
Lichtenbergstrasse 4, D-85747 Garching, Germany*

N. Khaneja

Division of Applied Sciences, Harvard University, Cambridge MA02138, USA

S.J. Glaser

*Department of Chemistry, Technical University Munich,
Lichtenbergstrasse 4, D-85747 Garching, Germany*

(Dated: February 1, 2008)

In this paper, we demonstrate that optimal control algorithms can be used to speed up the implementation of modules of quantum algorithms or quantum simulations in networks of coupled qubits. The gain is most prominent in realistic cases, where the qubits are not all mutually coupled. Thus the shortest times obtained depend on the coupling topology as well as on the characteristic ratio of the time scales for local controls *vs* non-local (*i.e.* coupling) evolutions in the specific experimental setting. Relating these minimal times to the number of qubits gives the tightest known upper bounds to the actual time complexity of the quantum modules. As will be shown, time complexity is a more realistic measure of the experimental cost than the usual gate complexity.

In the limit of fast local controls (as *e.g.* in NMR), time-optimised realisations are shown for the quantum Fourier transform (QFT) and the multiply controlled NOT-gate ($C^{n-1}NOT$) in various coupling topologies of n qubits. The speed-ups are substantial: in a chain of six qubits the quantum Fourier transform so far obtained by optimal control is more than eight times faster than the standard decomposition into controlled phase, Hadamard and SWAP gates, while the $C^{n-1}NOT$ -gate for completely coupled network of six qubits is nearly seven times faster.

PACS numbers: 03.67.-a, 03.67.Lx, 03.65.Yz, 03.67.Pp; 82.56.-b, 82.56.Jn, 82.56.Dj, 82.56.Fk

I. INTRODUCTION

A key motivation for using experimentally controllable quantum systems to perform computational tasks or to simulate the behaviour of other quantum systems [1, 2] roots in reducing the complexity of the problem when going from a classical setting to a quantum setting. The most prominent pioneering example being Shor's quantum algorithm of prime factorisation [3, 4]. While classical prime factorisation algorithms are of non-polynomial complexity NP [5], Shor's quantum algorithm brings it down into the class of polynomial complexity P . Another celebrated example is Grover's quantum search algorithm [6, 7], which allows for searching in an unstructured data base of n qubits with $N = 2^n$ items in $O(\sqrt{N})$ quantum steps instead of $O(N)$ classical ones.

As a matter of fact, many quantum algorithms can be subsumed as solving *hidden subgroup problems* in an efficient way [8]. In the abelian case, the speed-up hinges on the quantum Fourier transform (QFT): while the network complexity of the fast Fourier transform (FFT) for n classical bits is of the order $O(n2^n)$ [9, 10], the QFT for

n qubits shows a complexity of order $O(n^2)$. For implementing a quantum algorithm or a quantum simulation in an experimental setup, it is customary to break it into universal elementary quantum gates [11]. Common sets comprise *e.g.* (i) local operations such as the Hadamard gate, the phase gate and (ii) the entangling operations CNOT, controlled-phase gates, $\sqrt{\text{SWAP}}$, $i\text{SWAP}$ as well as (iii) the SWAP operation. The number of elementary gates required for implementing a quantum module then gives the network or gate complexity.

However, gate complexity often translates into too coarse an estimate for the actual time required to implement a quantum module (see *e.g.* [12, 13, 14]), in particular, if the time scales of a specific experimental setting have to be matched. Instead, effort has been taken to give upper bounds on the actual *time complexity* [15], which is a demanding goal from the algebraic point of view. With the time required for implementing a module in a specific experimental setting as the most realistic measure of cost, here we use methods of optimal control theory to find the minimum time by trying to solve the time-optimal control problem. The solution is hard to come by in general, so here we resort to numerical algorithms. The shortest times obtained depend on the coupling topology as well as on the characteristic ratio of the time scales for local controls *vs* non-local (*i.e.* coupling) evolutions and thus embrace the specific experimental setting. Relating these

*work presented in part at the QCBC 2004 in Glasgow

[†]Electronic address: tosh@ch.tum.de

minimal times to the number of qubits gives the tightest known upper bounds to the actual time complexity of the quantum modules in a realistic experimental setup.

Moreover, as will be discussed, in the generic case there is no simple one-to-one relation between time complexity and network complexity, because of different time-scales between local and non-local controls, different coupling topologies allowing for different degrees of parallelisation, and different types of coupling interactions matching different sets of elementary gates.

Thus here we leave the usual approach of decomposing gates into sets of discrete universal building blocks. Instead, the scope is to exploit the differential geometry of the unitary group for optimisation [16, 17] when using the power of quantum control in order to obtain constructive bounds to minimal time both as close to the experimental setting and as tight as possible. In the limit of zero cost for the fast local controls (as in NMR) compared to the slow coupling interactions, we give decompositions for the QFT and the multiply-controlled NOT-gate $C^{n-1}NOT$ that are dramatically faster than the fastest decompositions into standard gates known so far.

The paper is organised as follows: the first focus is on the fact that for time-optimal decompositions of a desired unitary gate into a sequence of evolutions of experimentally available controls the global phase may play a role. This is the case when *e.g.* there are different time scales for local versus non-local controls. However, global phases can readily be absorbed by shifting gradient flows from unitary to projective unitary groups. Then numerical time-optimal control provides the currently best upper bounds to the actual time complexity of quantum modules like the QFT or the $C^{n-1}NOT$ -gate in various coupling topologies of n qubit systems. Here we present examples with n up to seven. For $n \geq 3$, the resulting time complexities are bounded from above by *KAK*-type decompositions taken to sub-Riemannian regimes [18, 19, 20]. Finally we give an outlook generalising the methods developed from spin- to pseudo-spin systems.

Although the applications presented here refer to time-optimised quantum computing in the NMR-limit of fast local controls, the methods introduced are very general and apply to all systems whose dynamics can be cast into the closed form of finite-dimensional Lie algebras (to sufficient approximation).

II. CONTROLLABLE SYSTEMS

A. Spin- and Pseudo-Spin Systems

Here we address *fully controllable* [21, 22, 23, 24, 25, 26] quantum systems represented as spin- or pseudo-spin systems, *i.e.* those in which—neglecting decoherence—for any initial state represented by its density operator A , the entire unitary orbit $U(A) := \{UAU^{-1} \mid U \text{ unitary}\}$ can be reached [27]. In systems of n qubits (*e.g.* spins-

$\frac{1}{2}$), this is the case under the following mild conditions [16, 26, 28]: (1) the qubits have to be inequivalent *i.e.* distinguishable and selectively addressable, and (2) they have to be pairwise coupled (*e.g.* by Ising interactions), where the coupling topology may take the form of any connected graph.

B. Time Scales for Local and Non-Local Controls

Let the quantum system evolve in a time interval t_k under combinations of piece-wise constant control Hamiltonians $\{H_j\}$ and the drift H_d , *i.e.* the free-evolution Hamiltonian, according to

$$H^{(k)} = H_d + \sum_j u_j^{(k)} H_j^{(k)} . \quad (1)$$

In NMR spin dynamics [29], for instance, the local controls on qubit ℓ are represented by a linear combination of the Pauli matrices $\{\sigma_{\ell x}, \sigma_{\ell y}\}$. And the drift term is governed by the weak scalar couplings (reminiscent of Ising interactions)

$$H_d = \pi \sum_{\ell < m} J_{\ell m} \frac{1}{2} \sigma_{\ell z} \otimes \sigma_{mz} , \quad (2)$$

provided the couplings between spins are much smaller than the difference between the eigenfrequencies (shifts Ω) of the respective spins: $|J_{\ell m}| \ll |\Omega_\ell - \Omega_m|$. This is the case in heteronuclear spin systems. And in quantum control even the homonuclear ones can be designed such as to meet this greatly simplifying approximation [30].

For the system to be *fully controllable* in the sense outlined above, $\{H_d\} \cup \{H_j\}$ has to form a generating set of the Lie algebra $su(N)$ by way of the Lie bracket.

Often the time scale for local controls is considerably faster than for the costly slow coupling evolutions.

III. TIME-OPTIMAL QUANTUM CONTROL

In order to control a quantum system of n qubits (spins- $\frac{1}{2}$) such as to realise a quantum gate or module of some quantum algorithm given by the unitary propagator $U_G \in U(2^n)$ in minimal time, one has to decompose

$$U_G \sim U(T) = e^{-it_M H^{(M)}} \cdots e^{-it_k H^{(k)}} \cdots e^{-it_1 H^{(1)}} \quad (3)$$

—up to a global phase factor—into a *time-optimal sequence* ($T := \sum_k t_k \stackrel{!}{=} \min$) of evolutions under piecewise constant Hamiltonians $H^{(k)}$.

A. Relevance of Global Phases

However, as propagators generated by the traceless spin Hamiltonians are elements of the respective *special*

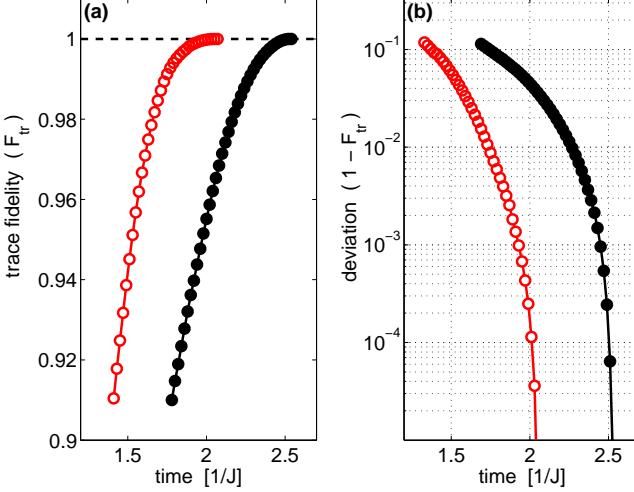


FIG. 1: Global phase dependence of the times needed to implement the 3-qubit QFT on a linear chain (L_3) of nearest-neighbour interactions with uniform weak scalar J -couplings. The right curves (\bullet) show the special unitary implementation of QFT with the smallest global phase $\phi_0 = \frac{1\pi}{16}$, where it takes $2.53 J^{-1}$ to reach a trace fidelity ≥ 0.99999 . The left curves (\circ) display the fastest QFT implementations obtained. They are attained with the global phase $\phi_1 = \frac{5\pi}{16}$. Trace fidelities ≥ 0.99999 are reached after $2.05 J^{-1}$. Times for local controls are assumed to be negligible in this limit matching the typical NMR scenario, where the time cost is determined by coupling evolutions. (a) gives the trace fidelities against time, while (b) shows the deviations from full fidelity in a semilogarithmic way.

unitary groups, the quantum gates U_G are realised by $U(T)$ just up to global phases ϕ_p

$$U_G = e^{-i\phi_p} U(T) ; \quad (4)$$

so $U_G \in U(N)$, while $U(T) \in SU(N)$. For n spins- $\frac{1}{2}$ read $N := 2^n$ henceforth. Note that with the centre of $SU(N)$ being

$$\mathbb{Z}_N := \{e^{i\frac{2\pi p}{N}} \mathbf{1}_N \mid p = 0, 1, \dots, N-1\} , \quad (5)$$

one has a choice of N such phases

$$\phi_p \in \{\phi_0 + \frac{2\pi p}{N} \mid p = 0, 1, \dots, N-1\} , \quad (6)$$

where ϕ_0 shall be the smallest angle $\phi_0 \in [0, \pi]$ so that $\det\{e^{i\phi_0} U_G\} = +1$. Although global phases are clearly immaterial to quantum evolutions $\rho_0 \mapsto U\rho_0U^{-1}$, it is important to note they do in fact contribute substantially to the over-all time needed to implement U_G : consider, e.g.,

$$e^{-i\frac{\pi}{2}\sigma_{\ell z} \otimes \sigma_{mz}} = e^{i\frac{\pi}{2}} e^{-i\frac{\pi}{2}(\sigma_{\ell z} \otimes \mathbf{1} + \mathbf{1} \otimes \sigma_{mz})} , \quad (7)$$

where the non-scalar part of the right-hand-side can be realised solely by (fast) local controls, whereas the left-hand-side hinges on nothing but (slow) coupling evolution.

In Fig. 1 this is further illustrated for the 3-qubit QFT implemented on a chain of three spins connected by nearest-neighbour interactions of weak scalar coupling in the NMR limit of zero time cost for the fast local controls.

B. Optimal Control on Projective Groups

For a given unitary quantum gate U_G and propagators $U = U(t)$ describing the evolution of the quantum system, there are the two geometric tasks, one that explicitly carries the phase, while the other one automatically absorbs it as desired:

- (1) minimise the distance $\|U - U_G\|_2$ by maximising $\Phi_1 := \text{Re } \text{tr}\{U_G^\dagger U\}$;
- (2) minimise the angle $\angle(U, U_G) \bmod(\pi)$ by maximising $\Phi_2 := |\text{tr}\{U_G^\dagger U\}|^2$.

(1) In terms of control theory, the first task is to maximise the quality functional $\Phi_1[U(t)] = \text{Re } \text{tr}\{U_G^\dagger U(T)\}$ with $0 \leq t \leq T$ subject to the equation of motion $\dot{U}(t) = -iHU(t)$ (with $H = H_d + \sum_j u_j H_j$) and the initial condition $U(0) = \mathbf{1}$, whereas the final condition $U(T)$ is free at an appropriately fixed final time T (vide infra). As usual, the problem is readily solved by introducing the operator-valued Lagrange multiplier $\lambda(t)$ satisfying $\dot{\lambda}(t) = -iH\lambda(t)$ and a scalar-valued Hamiltonian function

$$h(U(t_k)) = \text{Re } \text{tr}\left\{\lambda^\dagger(t_k) \left(-i(H_d + \sum_j u_j H_j)\right) U(t_k)\right\} . \quad (8)$$

Then, Pontryagin's maximum principle [31] may be exploited in a quantum setting [32, 33] to require

$$\frac{\partial h(U(t_k))}{\partial u_j} \equiv -\text{Im } \text{tr}\{\lambda^\dagger(t_k) H_j U(t_k)\} \stackrel{!}{=} 0 \quad (9)$$

as well as the final condition for the adjoint system

$$\lambda(T) = -\frac{\partial \Phi_1(T)}{\partial U(T)} = -U_G \quad (10)$$

thus allowing to implement a gradient-flow based recursion [33]. For the amplitude of the j th control in iteration $r+1$ at time interval t_k one finds with α as a suitably chosen step size

$$u_j^{(r+1)}(t_k) = u_j^{(r)}(t_k) + \alpha \frac{\partial h(U(t_k))}{\partial u_j} . \quad (11)$$

The procedure is then repeated for a set of decreasing final times T up to a minimal time τ still allowing to get sufficient fidelity (compare Fig. 1).

- (2) The second task amounts to maximising $\Phi_2[U(t)] = |\text{tr}\{U_G^\dagger U(T)\}|^2$, which is equivalent to the square of the

trace fidelity and is easy to handle by gradient-flow methods. This problem, however, can readily be reduced to task (1): observe that to $U \in SU(N)$,

$$\hat{U} := U^* \otimes U \quad (12)$$

is a representation of the corresponding element of the *projective special unitary group*

$$PSU(N) \xrightarrow{\text{iso}} \frac{SU(N)}{\mathbb{Z}_N} \xrightarrow{\text{iso}} \frac{U(N)}{U(1)} \quad (13)$$

embedded in $SU(N^2)$. Hence this representation is highly reducible yet very convenient, because

$$\Phi_1[\hat{U}(t)] = \text{Re } \text{tr}\{\hat{U}_G^\dagger \hat{U}(T)\} = |\text{tr}\{U_G^\dagger U(T)\}|^2 = \Phi_2[U(t)]. \quad (14)$$

Hence one may adopt the previous results to obtain the gradient flow on $PSU(N)$ just by using

$$\frac{\partial h(\hat{U}(t_k))}{\partial u_j} \equiv -2 \text{Im} (\text{tr}\{\lambda^t(t_k) H_j^t U^*(t_k)\} \cdot \text{tr}\{\lambda(t_k)^\dagger U(t_k)\}) \quad (15)$$

in Eqn. 11. Thus an explicit tensor product never enters the algorithm. And the final condition of the adjoint system does not require any prior knowledge or screening of the global phase ultimately giving the fastest implementation as has been the case in previous settings, *e.g.* [34], because embedding $PSU(N)$ in $SU(N^2)$ enforces a global phase of zero. Absorbing the phases cuts the number of computations for n -qubit systems by a factor $N = 2^n$.

Having reduced task (2) to task (1) also saves all the convergence and step-size considerations [17] from $SU(N^2)$ to apply to $PSU(N)$.

With these stipulations, the Hamiltonians H_k according to Eqn. 1, and the numbering as in Eqn. 3, the iterations r of Eqn. 11 can be used in the following algorithmic scheme [33]:

1. set initial controls $u_j^{(0)}(t_k)$ for all times t_k with $k = 1, 2, \dots, M$ at random or by guess;
2. starting from $U_0 = \mathbb{1}$, calculate for all t_1, t_2, \dots, t_k the forward-propagation

$$U^{(r)}(t_k) = e^{-i(t_k-t_{k-1})H_k^{(r)}} e^{-i(t_{k-1}-t_{k-2})H_{k-1}^{(r)}} \dots \\ \times e^{-i(t_1-t_0)H_1^{(r)}} U_0 \quad (16)$$

3. likewise, starting with $T = t_M$ and $\lambda(T)$ from Eqn. 10, compute for all t_M, t_{M-1}, \dots, t_k the back-propagation

$$\lambda^{(r)}(t_k) = e^{i(t_k-t_{k-1})H_k^{(r)}} e^{i(t_{k+1}-t_k)H_{k+1}^{(r)}} \dots \\ \times e^{i(t_M-t_{M-1})H_M^{(r)}} \lambda(T) \quad (17)$$

4. calculate $\frac{\partial h(U(t_k))}{\partial u_j}$ according to Eqn. 9;
5. with $u_j^{(r+1)}(t_k)$ from Eqn. 11 update all the piecewise Hamiltonians to $H_k^{(r+1)}$ and return to step 2.

Topology	K_4	S_4	C_4	L_4
$\tau [1/J]$	1.75	3.05	3.11	3.15

FIG. 2: Four ordered connected graphs with 4 vertices representing the topology of pairwise couplings (edges) between 4 qubits (vertices). Times given are for the shortest QFT-realisations obtained by numerical time-optimal control rounded to 0.01 J^{-1} .

IV. APPLICATIONS

For simplicity, the coupling strengths in all the subsequent examples are assumed uniform, thus enabling to give the times in units of J^{-1} . However, all our algorithms can equally well cope with non-uniform coupling constants directly matching the experimental settings.

A. Towards a Time-Optimal Quantum Fourier Transform

The quantum Fourier transform (QFT) is central to all quantum algorithms of abelian hidden subgroup type [35, 36]. The time required to implement this module in n -qubit systems clearly depends on the topology of the coupling interactions.

Fig. 2 shows some of the topologies for the couplings of four qubits and the respective times (best numerical results from optimal control) for implementing the 4-qubit QFT. Clearly, the complete coupling topology corresponds to the maximal graph K_n and thus allows for the fastest implementation, while the chain of nearest-neighbour interactions L_n is the minimal connected graph entailing the slowest implementation. Note, however, that the minimal times also depend on the ordering in the graph, because permutations (carried out by transpositions) may call for timewise costly SWAPs.

The decomposition into standard gates (controlled phase gate, Hadamard, and SWAP) can readily be made time-optimal only in complete coupling topologies (K_n). There the minimal time can easily be expressed in units of J^{-1} as a function of the number qubits (compare [37, 38])

$$\tau(n) = \frac{1}{4}(n+3) \quad , \quad (18)$$

where the constant covers the final SWAP.

However, as is shown in Fig. 3 and Tab. I (note the details in the table caption), in linear spin chains (L_n) with nearest-neighbour Ising interactions, time-optimal control provides a decomposition of the QFT that is much

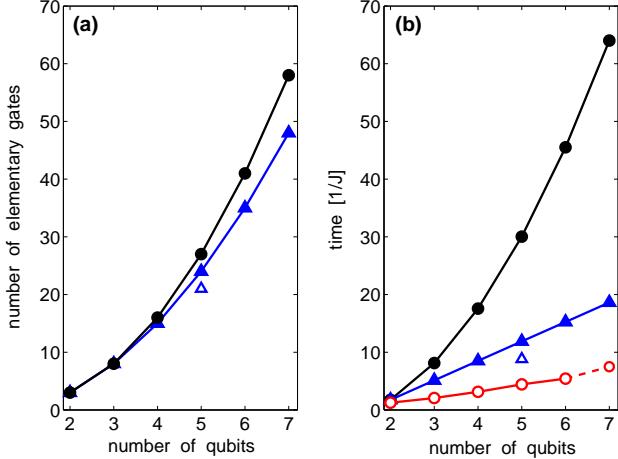


FIG. 3: (a) Gate complexity of the QFT in linear coupling topologies L_n . Standard-gate decomposition (\bullet) [39] and optimised scalable gate decomposition (\blacktriangle) [40]. (b) Time complexity of the QFT in linear coupling topologies. Upper traces give analytical times associated with the decompositions of part (a): standard-gate decompositions (\bullet) [39] and optimised scalable gate decompositions (\blacktriangle) [40]; (Δ) gives a special (*i.e.* non scalable) five-qubit decomposition into standard gates obtained by simulated annealing [40]. Lowest trace: speed-up by time-optimal control with shortest numerical realisations obtained (\circ) rounded to $0.01 J^{-1}$. Further details in Tab. I. (At 7 qubits current decompositions show a trace fidelity of ~ 0.99 and thus have not enough significant digits to be included in the subsequent table.)

TABLE I: Speed-up of the Quantum Fourier Transform on Linear Spin Chains, L_n

qubits	stand. QFT ^a		Blais ^b		best results ^c	speed-ups
	$\tau [1/J]^d$	$\tau [1/J]^d$	$\tau [1/J]^d$	stand.		
2	1.75	1.75	1.25	1.40	1.40	
3	8.13	5.13	2.05	3.94	2.50	
4	17.56	8.50	3.15	5.58	2.70	
5	30.03	11.88(8.81)	4.44	6.77	2.67(1.98)	
6	45.52	15.25	5.43	8.38	2.81	

^aanalytical times for decomposition into standard gates [39]

^b[40] in brackets: the non-scalable special 5-qubit QFT

^cupper bounds to minimal time for achieving a trace fidelity of ≥ 0.99999 by numerical optimal control

^dtimes τ are rounded to $0.01 J^{-1}$

faster than the corresponding decomposition into standard gates would impose: in six qubits, for instance, the speed-up is more than eight-fold and in seven qubits approximately nine-fold.

For a fair comparison, however, note that Blais [40] permutes output qubits for saving SWAPS. However, searching through $n!$ permutations is beyond our cpu-time credits, but may provide even faster realisations in the future.

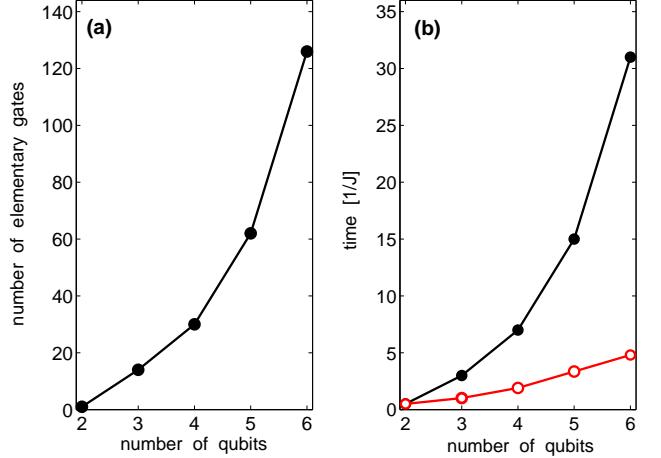


FIG. 4: (a) Network complexity of the C^{n-1} NOT-gate on complete coupling topologies K_n [41]. (b) Time complexity of the C^{n-1} NOT-gate on complete coupling topologies. Upper trace: analytical times for decomposition into standard gates (\bullet) [41]. Lower trace: speed-up by time-optimal control with shortest times (\circ) currently needed for realising C^{n-1} NOT by numerical control rounded to $0.01 J^{-1}$.

TABLE II: Speed-up for the C^{n-1} NOT-Gate in Complete Coupling Topologies of n Qubits, K_n

qubits	stand. decomposition ^a $\tau [1/J]^c$	best results ^b $\tau [1/J]^c$	speed-up
2	0.5	0.50	1.00
3	3.0	1.01	2.97
4	7.0	1.90	3.68
5	15.0	3.37	4.45
6	31.0	(4.59)	(6.75)

^aBarenco *et al.* [41]

^bupper bounds to minimal time for trace fidelities ≥ 0.99999 (for 6 qubits currently: ≥ 0.999) by numerical optimal control

^ctimes τ are rounded to $0.01 J^{-1}$

B. Towards a Time-Optimal C^{n-1} NOT

Likewise, one may strive to implement the C^{n-1} NOT-gate in a time-optimal way. In a complete coupling topology of n qubits, the algorithmic complexity was described by Barenco *et al.* [41] as increasing exponentially up to six qubits, whereas the increase from seven qubits onwards was said to be quadratic. Again, time-optimal control provides a dramatic speed-up in this case as well, see Fig. 4 and Tab. II as well as the controls in Fig. 5.

C. Beyond Spins: Controlling Coupled Charge Qubits in Josephson Devices

Obviously the optimal control methods presented thus far can be generalised such as to hold for systems with finite degrees of freedom allowing for a pseudospin for-

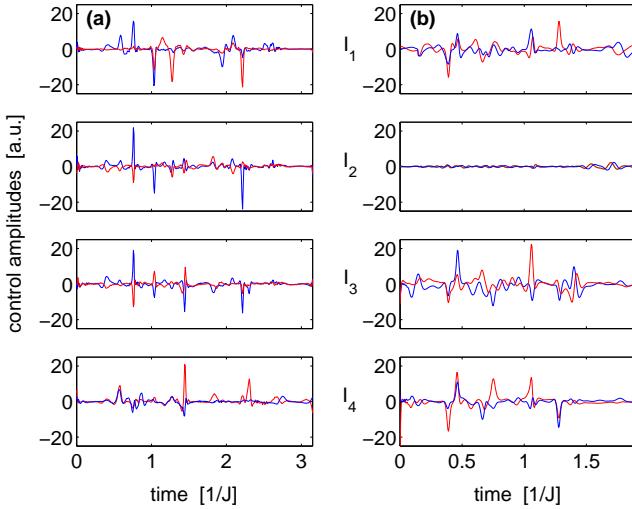


FIG. 5: Time course of controls for the shortest realisations obtained for the following quantum modules: (a) the QFT on a linear coupled four-qubit system (L_4); (b) the $c^3\text{NOT}$ -gate on a fully coupled four-qubit system K_4 . Traces in blue: amplitudes for $\sigma_{\ell x}$ -controls (x -pulses); red: amplitudes for $\sigma_{\ell y}$ -controls (y -pulses) on the spins $\ell = 1, 2, 3, 4$.

mulation in terms of closed Lie algebras. Suffice it to mention the standard CNOT-gate can be realised in two coupled charge qubits of a solid-state Josephson device some five times faster than in the pioneering setting of Nakamura [42]. Yet one easily obtains a trace fidelity beyond 0.99999 as will be shown elsewhere. With the same fidelities one finds realisations of the TOFFOLI-gate in three linearly coupled charge qubits that are some nine times faster than by standard gate decomposition.

V. DISCUSSION

The goal is to extend the optimal control methods to larger modules of quantum algorithms or simulations in order to implement them both in a time-optimal and experimentally robust way. Thus the growing set of numerical examples will hopefully provide inspiration to understand time-optimal steerings of quantum systems algebraically, which, however, seems very demanding in the cases presented here (compare Fig. 5). In other instances such as for the propagator

$$U(t) = e^{-i\pi Jt \left(\frac{1}{2}\sigma_{1z} \otimes \sigma_{2z} \otimes \sigma_{3z}\right)}, \quad (19)$$

the theory is fully understood, and the predictions based on sub-Riemannian geodesics [20] perfectly match (i) the time-complexity as well as (ii) the actual time course for the controls [33] for all $\pi Jt \in [0, \frac{\pi}{2}]$.

Along these lines, the above controls may finally trigger a theoretical understanding. The ultimate challenge then is to extract a principle for a *scalable* control scheme from the set of numerical examples.

VI. CONCLUSION

Here we have left the usual approach of decomposing quantum modules into sets of discrete building blocks, such as elementary universal quantum gates thus expressing the cost as algorithmic network complexity. Instead we proposed to refer to *time complexity* as the experimentally relevant cost: it allows for exploiting the continuous differential geometry of the unitary Lie-groups as well as the power of quantum control for getting constructive upper bounds to the time complexity both perfectly matching the experimental setting while being as tight as possible, in particular when local and non-local operations are of different time scale. In the limit of zero cost for the fast local controls we gave decompositions for the QFT and the multiply-controlled NOT-gate $C^{n-1}\text{NOT}$ that are dramatically faster than the best decompositions into standard gates known so far would impose. However, there is no guarantee the ultimate time optimum is attained, also because permutations of the qubits may give further improvement.

The approach also clearly shows that in the generic case there is no simple one-to-one relation between time complexity and network complexity. This is for very practical reasons: typically (1) not all the elementary gates are of the same time cost, but each experimental implementation comes with its characteristic ratio of times required for local *vs* non-local (coupling) operations; (2) not all the elementary gates have to be performed sequentially, but can be rearranged so that some of the commuting operations (*e.g.* controlled phase gates between several qubits) or operations in disjoint subspaces can be parallelised; (3) the coupling topology between the qubits does not have to form a complete graph (K_n) but may be just a connected subgraph, and each graph comes with a specific potential of parallelising timewise costly interactions; this is demonstrated for the QFT on complete coupling topologies K_n versus the linear coupling topology L_n , where the parallel performance of controlled phase gates [40] reduces quadratic time complexity to linear complexity, which, however, can be further speeded up by time-optimal control; (4) the experimental setting with its specific type and individual strengths of coupling interaction (*e.g.* Ising or Heisenberg-XY or XYZ type) related to the choice of universal gates for the network decomposition may introduce some arbitrariness.

It is for these very reasons that time complexity is the more realistic measure of the experimentally relevant cost than network complexity is.

VII. OUTLOOK

Although extrapolation may be premature, it is fair to anticipate that in systems of some 20 qubits network decompositions will often become impractical. Thus time-optimal decompositions into controls actually avail-

able in the experimental setting promise to widen the range of experimentally accessible tasks significantly and will prove useful in many experimental implementations. Moreover, analysing the topology-dependence of minimal times while allowing for non-uniform coupling strengths will contribute valuable guidelines for designing optimised architectures of quantum computational hardware.

By parallelising routines the results are currently being extended to more qubits so that time complexities can be deduced from fitting times against number of qubits with confidence.

Acknowledgments

This work was supported in part by *Deutsche Forschungsgemeinschaft*, DFG, in the grant GI 203/4-2 and in the incentive SPP 1078 (*Schwerpunkt-Programm ‘Quanteninformationsverarbeitung’, QIV*). Encouraging discussion with Ivan Deutsch and Andrew Landahl at the QCMC 2004 is gratefully acknowledged.

-
- [1] R. P. Feynman, Int. J. Theo. Phys. **21**, 467 (1982).
- [2] R. P. Feynman, *Feynman Lectures on Computation* (Perseus Books, Reading, MA., 1996).
- [3] P. W. Shor, in *Proceedings of the Symposium on the Foundations of Computer Science, 1994, Los Alamitos, California* (IEEE Computer Society Press, New York, 1994), pp. 124–134.
- [4] P. W. Shor, SIAM J. Comput. **26**, 1484 (1997).
- [5] C. H. Papadimitriou, *Computational Complexity* (Addison Wesley, Reading, MA., 1995).
- [6] L. K. Grover, in *Proceedings of the 28th Annual Symposium on the Theory of Computing, 1996, Philadelphia, Pennsylvania* (ACM Press, New York, 1996), pp. 212–218.
- [7] L. K. Grover, Phys. Rev. Lett. **79**, 325 (1997).
- [8] M. Ettinger, P. Høyer, and E. Knill, Inf. Process. Lett. **91**, 43 (2004).
- [9] J. W. Cooley and J. W. Tukey, Math. Comput. **19**, 297 (1965).
- [10] T. Beth, *Verfahren der schnellen Fourier-Transfomation* (Teubner, Stuttgart, 1984).
- [11] D. Deutsch, Proc. Royal Soc. London A **400**, 97 (1985).
- [12] G. Vidal, K. Hammerer, and J. I. Cirac, Phys. Rev. Lett. **88**, 237902 (2002).
- [13] A. M. Childs, H. L. Haselgrave, and M. A. Nielsen, Phys. Rev. A **68**, 052311 (2003).
- [14] R. Zeier, M. Grassl, and T. Beth, Phys. Rev. A **70**, 032319 (2004).
- [15] P. Wocjan, D. Janzing, and T. Beth, Quant. Inf. Comput. **2**, 117 (2002).
- [16] S. J. Glaser, T. Schulte-Herbrüggen, M. Sieveking, O. Schedetzky, N. C. Nielsen, O. W. Sørensen, and C. Griesinger, Science **280**, 421 (1998).
- [17] U. Helmke, K. Hüper, J. B. Moore, and T. Schulte-Herbrüggen, J. Global Optim. **23**, 283 (2002).
- [18] N. Khaneja and S. J. Glaser, Chem. Phys. **267**, 11 (2001).
- [19] N. Khaneja, R. Brockett, and S. J. Glaser, Phys. Rev. A **63**, 032308 (2001).
- [20] N. Khaneja, S. J. Glaser, and R. Brockett, Phys. Rev. A **65**, 032301 (2002).
- [21] V. Jurdjevic and H. Sussmann, J. Diff. Equat. **12**, 313 (1972).
- [22] H. Sussmann and V. Jurdjevic, J. Diff. Equat. **12**, 95 (1972).
- [23] R. W. Brockett, SIAM J. Control **10**, 265 (1972).
- [24] R. W. Brockett, SIAM J. Appl. Math. **25**, 213 (1972).
- [25] W. M. Boothby and E. N. Wilson, SIAM J. Control Op. tim. **17**, 212 (1979).
- [26] T. Schulte-Herbrüggen, *Aspects and Prospects of High-Resolution NMR* (PhD Thesis, Diss-ETH 12752, Zürich, 1998).
- [27] F. Albertini and D. D’Alessandro, IEEE Trans. Automat. Control **48**, 1399 (2003).
- [28] T. Schulte-Herbrüggen, K. Hüper, U. Helmke, and S. J. Glaser, *Applications of Geometric Algebra in Computer Science and Engineering* (Birkhäuser, Boston, 2002), chap. Geometry of Quantum Computing by Hamiltonian Dynamics of Spin Ensembles, pp. 271–283.
- [29] R. R. Ernst, G. Bodenhausen, and A. Wokaun, *Principles of Nuclear Magnetic Resonance in One and Two Dimensions* (Clarendon Press, Oxford, 1987).
- [30] R. Marx, A. F. Fahmy, J. M. Myers, W. Bermel, and S. J. Glaser, Phys. Rev. A **62**, 012310 (2000).
- [31] L. S. Pontryagin, V. G. Bol’tanskii, R. S. Gamkrelidze, and E. F. Mischenko, *The Mathematical Theory of Optimal Processes* (Pergamon Press, New York, 1964).
- [32] A. G. Butkovskiy and Y. I. Samoilenco, *Control of Quantum-Mechanical Processes and Systems* (Kluwer, Dordrecht, 1990).
- [33] N. Khaneja, T. Reiss, C. Kehlet, T. Schulte-Herbrüggen, and S. J. Glaser, J. Magn. Reson. **172**, 296 (2005).
- [34] J. Wesenberg, Phys. Rev. A **69**, 042323 (2004), see in particular Eqn. 14 in quant-ph/0312076.
- [35] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge (UK), 2000).
- [36] G. Alber, T. Beth, M. Horodecki, P. Horodecki, R. Horodecki, M. Rötteler, H. Weinfurter, R. Werner, and A. Zeilinger, *Quantum Information: an Introduction to Basic Concepts and Experiments (Springer Tracts in Modern Physics Vol. 173)* (Springer, Heidelberg, 2000).
- [37] M. D. Price, T. F. Havel, and D. J. Cory, New J. Phys. **2**, 10.1 (2000), URL <http://www.iop.org/EJ/article/1367-2630/2/1/10/nj0110.html>.
- [38] K. Dorai and D. Suter (2002), quant-ph/0211030.
- [39] A. Saito, K. Kioi, Y. Akagi, N. Hashizume, and K. Ohta (2000), quant-ph/0001113.
- [40] A. Blais, Phys. Rev. A **64**, 022312 (2001).
- [41] A. Barenco, C. H. Bennett, R. Cleve, D. P. DiVincenzo, N. Margolus, P. Shor, T. Sleator, J. A. Smolin, and H. Weinfurter, Phys. Rev. A **52**, 3457 (1995).
- [42] T. Yamamoto, Y. A. Pashkin, O. Astaviev, Y. Nakamura, and J. S. Tsai, Nature (London) **425**, 941 (2003).